



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:15 AM UTC

PDB ID : 8DYU / pdb_00008dyu
EMDB ID : EMD-27782
Title : Structure of human cytoplasmic dynein-1 bound to two Lis1 proteins
Authors : Reimer, J.M.; DeSantis, M.; Reck-Peterson, S.L.; Leschziner, A.E.
Deposited on : 2022-08-05
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

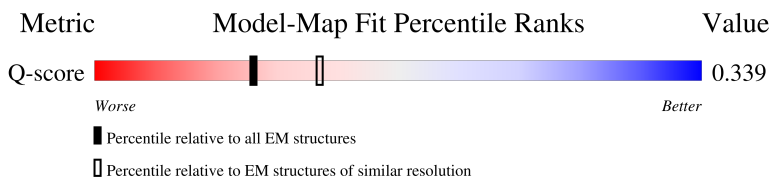
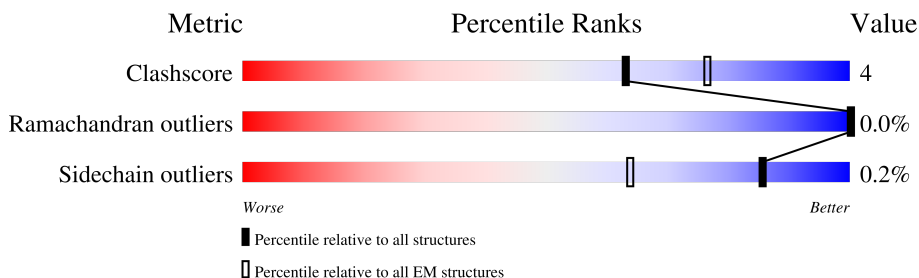
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3328	
2	B	411	
2	C	411	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48226 atoms, of which 23616 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2562	Total	C	H	N	O	S	0	0
			38760	12606	19046	3405	3601	102		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1319	GLY	-	expression tag	UNP Q14204

- Molecule 2 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	306	Total	C	H	N	O	S	0	0
			4721	1522	2309	422	448	20		
2	C	306	Total	C	H	N	O	S	0	0
			4585	1497	2213	413	442	20		

There are 4 discrepancies between the modelled and reference sequences:

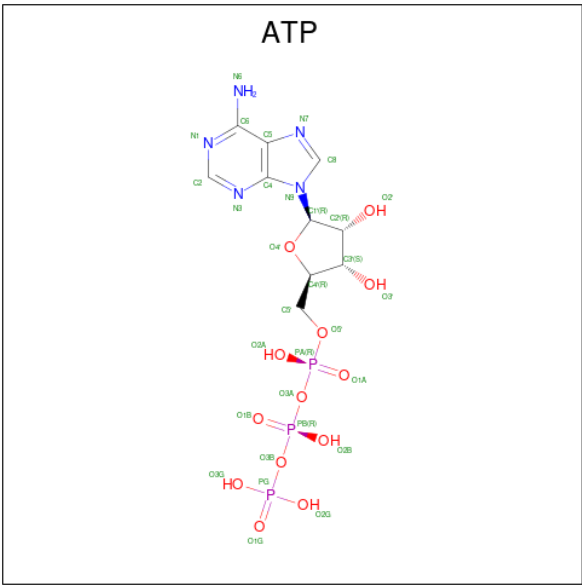
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P43034
B	1	SER	-	expression tag	UNP P43034
C	0	GLY	-	expression tag	UNP P43034
C	1	SER	-	expression tag	UNP P43034

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



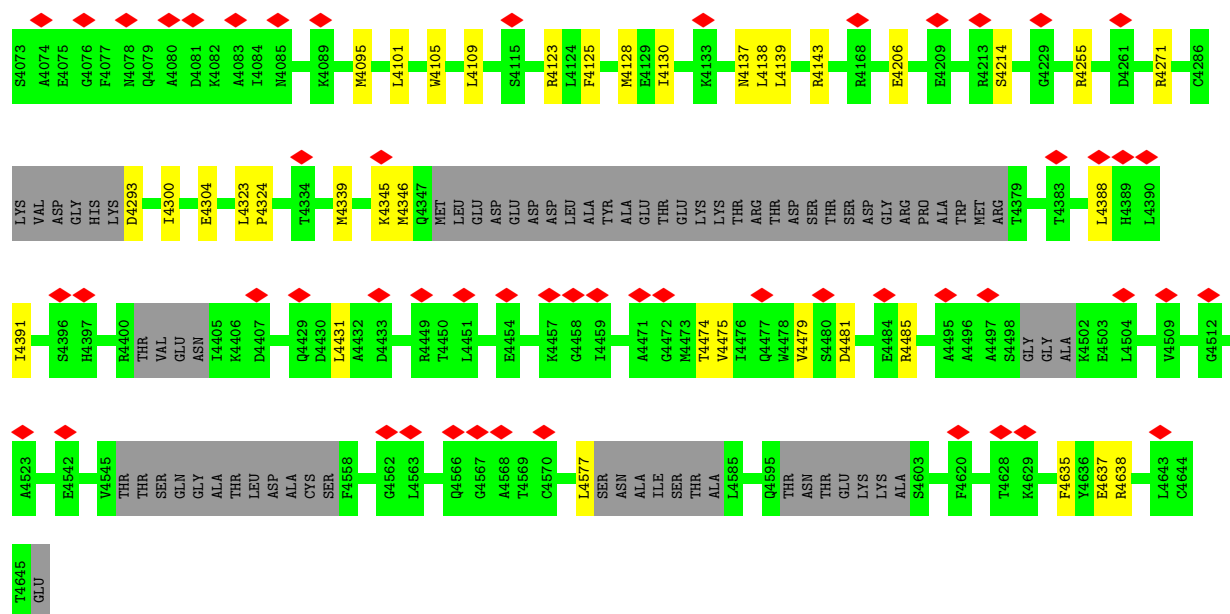
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
3	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
3	A	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

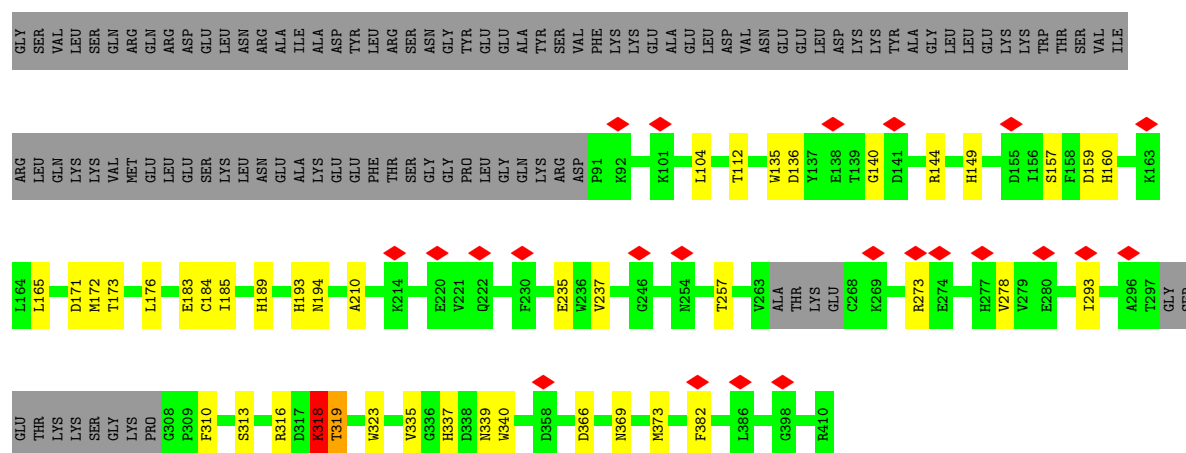


Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

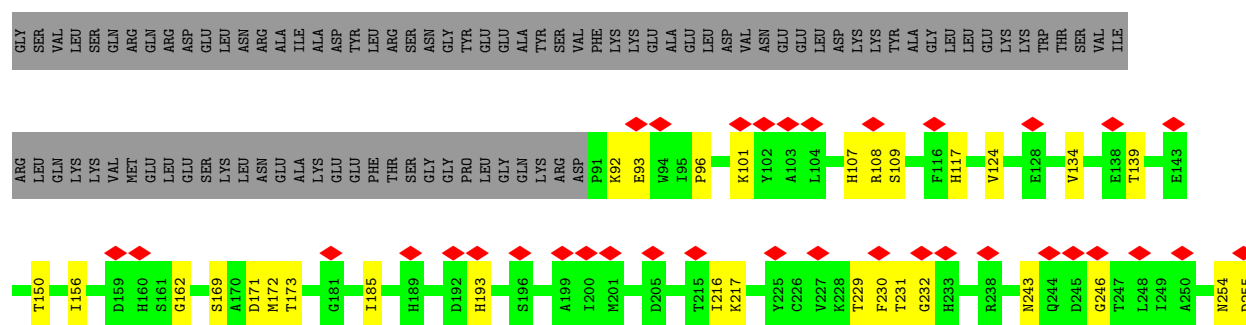
E2078	E2087	L2090	S2095	E2106	R2107	I2111	LYS	ARG	GLU	LYS	E2313	N2314	GLU	GLU	ARG	GLY	GLY	GLU	ILE	K2128	Q2139	D2153	F2158	E2180	Y2190	D2195	E2198	W2202	W2203	V2207	L2210	Y2211	W2221	W2222	S2231	L2237	L2268		
N2271	T2272	R2273	V2291	R2292	K2297	W2300	V2307	E2313	N2314	L2315	T2326	N2338	E2344	L2348	T2352	N2377	L2382	E2389	GLY	ASP	GLU	ALA	GLN	ARG	ARG	LYS	LYS	GLU	ASP	GLU	GLY	GLU	ALA	Q2416	M2423	L2432			
E2438	L2443	E2444	M2447	D2448	R2453	L2458	M2461	L2462	H2463	Q2464	R2492	A2497	L2498	L2499	D2505	L2514	Y2517	T2521	T2522	E2544	A2563	D2573	R2576	H2577	L2580	L2581	T2582	L2591	C2594	F2606	R2610	D2614	V2617	S2623					
E2629	F2635	N2646	Q2654	L2655	G2656	L2668	F2669	D2670	K2673	Y2674	G2675	R2694	D2697	Q2698	T2699	R2705	C2712	R2720	V2733	L2752	E2782	T2785	Q2786	D2787	R2804	L2813	L2816	R2823	A2829	D2840	E2841	R2844	E2848	N2849	T2851	T2852			
L2855	P2859	ASN	ILE	ASP	ARG	K2865	I2871	D2880	Y2892	R2896	E2904	F2912	N2913	E2914	V2915	H2918	V2919	I2922	L2934	K2943	V2950	K2962	V2963	H2964	R2965	K2966	Y2967	T2968	D2971	F2972	D2973	E2974	D2975	V2979	L2980	F2992	I2993	E2996	L3000
D3001	S3002	G3003	E3006	G3019	G3023	Q3032	C3033	K3034	E3040	G3041	D3045	K3068	S3071	S3072	E3073	R3078	N3087	D3096	K3097	T3110	D3114	N3119	D3124	K3132	R3140	L3154	H3155	A3162	R3167	I3171	K3174	D3178	K3190	Q3198					
N3202	L3205	R3206	K3207	V3212	D3213	Q3214	VAL	GLU	LEU	ARG	ASP	LEU	ARG	ILE	LYS	SER	GLN	LEU	VAL	ALA	ALA	ASN	ASP	LYS	LYS	MET	VAL	LYS	VAL	GLN	ASP	GLN	GLU	LYS	VAL	GLN	LEU		
HIS	LYS	GLN	LEU	GLY	VAL	ILE	ALA	ASP	LYS	GLN	MET	LYS	GLN	SER	VAL	VAL	LYS	ARG	GLU	ASP	ILE	LEU	ASP	LYS	VAL	VAL	LYS	ASP	LYS	TRP	LYS	ASP	THR	THR	THR	THR	THR		
CYS	LEU	LEU	LEU	CYS	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
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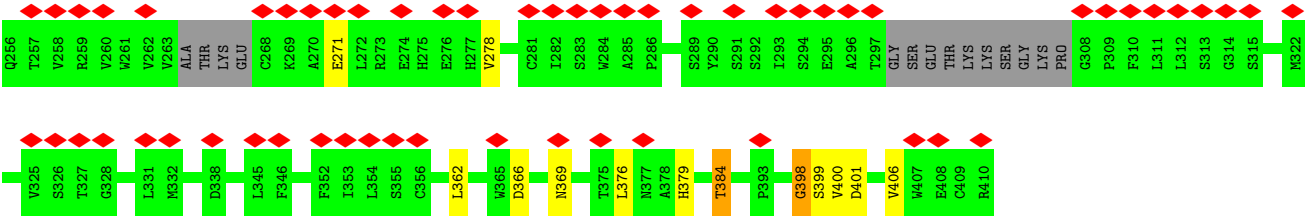


• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta



• Molecule 2: Platelet-activating factor acetylhydrolase IB subunit beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.916	Depositor
Minimum map value	-0.528	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.19	Depositor
Map size ($\text{\AA}$)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.20	0/20129	0.45	4/27375 (0.0%)
2	B	0.33	1/2476 (0.0%)	0.65	7/3358 (0.2%)
2	C	0.36	0/2436	0.63	2/3313 (0.1%)
All	All	0.24	1/25041 (0.0%)	0.49	13/34046 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	278	VAL	C-O	-8.47	1.14	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	112	THR	CA-C-O	-8.35	110.07	119.67
2	C	384	THR	CA-C-O	-8.16	112.49	120.90
2	B	319	THR	CB-CA-C	-7.77	98.88	110.62
2	B	278	VAL	CA-C-O	-6.87	112.20	120.78
2	B	318	LYS	N-CA-C	-6.46	105.34	113.23
1	A	3765	THR	N-CA-C	-6.32	104.39	111.28
2	C	398	GLY	CA-C-O	-6.02	115.09	120.75
2	B	144	ARG	CA-C-O	-5.47	115.25	120.94
1	A	3772	ASN	CB-CA-C	-5.46	100.70	110.70
2	B	278	VAL	CA-C-N	5.20	129.88	123.12
2	B	278	VAL	C-N-CA	5.20	129.88	123.12
1	A	3772	ASN	N-CA-CB	5.16	117.89	110.20
1	A	3758	GLY	CA-C-O	-5.04	116.11	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19714	19046	19054	150	0
2	B	2412	2309	2309	30	0
2	C	2372	2213	2224	28	0
3	A	81	36	36	2	0
4	A	31	12	12	0	0
All	All	24610	23616	23635	200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3770:LEU:HG	1:A:3770:LEU:O	1.84	0.78
1:A:4206:GLU:OE2	1:A:4255:ARG:NH1	2.21	0.74
1:A:2447:MET:HE1	1:A:2733:VAL:HG21	1.70	0.73
2:C:379:HIS:CD2	2:C:399:SER:OG	2.44	0.70
1:A:3198:GLN:OE1	1:A:3202:ASN:ND2	2.25	0.69
1:A:2423:MET:HE1	1:A:2462:LEU:HD22	1.75	0.69
1:A:4271:ARG:NH1	1:A:4637:GLU:OE1	2.29	0.66
1:A:1861:MET:HB3	1:A:1864:ALA:HB3	1.78	0.65
2:C:399:SER:C	2:C:401:ASP:H	2.06	0.64
1:A:2848:GLU:O	1:A:2852:THR:HG23	1.98	0.64
1:A:2979:VAL:HG11	1:A:2992:PHE:HZ	1.63	0.64
1:A:2025:ARG:NH2	1:A:2313:GLU:OE1	2.31	0.64
1:A:3881:ILE:HG23	1:A:4339:MET:HE1	1.79	0.63
1:A:2492:ARG:NH2	1:A:2544:GLU:OE2	2.31	0.63
1:A:1861:MET:HG3	1:A:1862:ALA:H	1.63	0.62
1:A:3580:LEU:HD13	1:A:3600:ILE:HD12	1.81	0.62
1:A:1885:THR:HG22	1:A:1889:TYR:CE2	2.35	0.62
1:A:3749:LEU:CD2	1:A:3770:LEU:HD12	2.29	0.62
1:A:3756:VAL:HG21	1:A:3766:ILE:HD11	1.81	0.62
2:C:255:ASP:O	2:C:255:ASP:OD1	2.17	0.62
1:A:2823:ARG:NH1	1:A:2865:LYS:O	2.32	0.62
1:A:3656:THR:CB	2:B:193:HIS:CD2	2.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:LYS:N	2:C:406:VAL:O	2.33	0.61
1:A:2694:ARG:O	1:A:2698:GLN:N	2.33	0.61
1:A:3478:LEU:HD22	1:A:3767:ILE:HG23	1.82	0.61
1:A:3656:THR:CB	2:B:193:HIS:HD2	2.13	0.61
2:B:257:THR:HG23	2:B:273:ARG:CG	2.31	0.59
1:A:3588:LEU:HG	1:A:3696:VAL:HG11	1.84	0.59
1:A:2447:MET:CE	1:A:2733:VAL:HG21	2.32	0.59
1:A:2594:CYS:HB3	1:A:2712:CYS:SG	2.43	0.59
1:A:1939:GLN:OE1	1:A:1939:GLN:N	2.35	0.58
1:A:4577:LEU:HD13	1:A:4635:PHE:CE1	2.39	0.58
1:A:1738:TYR:HE2	1:A:1792:LEU:HD21	1.69	0.58
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.30	0.58
2:B:235:GLU:N	2:B:235:GLU:OE1	2.37	0.58
1:A:2979:VAL:HG21	1:A:2992:PHE:CE1	2.39	0.57
2:B:104:LEU:HD13	2:B:135:TRP:CE3	2.40	0.57
1:A:2594:CYS:SG	1:A:2733:VAL:CG1	2.93	0.57
1:A:3212:VAL:HG22	1:A:3479:LEU:HD11	1.87	0.56
1:A:2190:TYR:O	1:A:2377:ASN:ND2	2.37	0.56
1:A:4035:VAL:O	1:A:4123:ARG:NH2	2.38	0.56
1:A:2313:GLU:OE2	1:A:2352:THR:OG1	2.24	0.56
1:A:3167:ARG:NH2	1:A:3519:TYR:OH	2.38	0.56
2:B:257:THR:HG23	2:B:273:ARG:HG2	1.87	0.55
1:A:3500:MET:HA	1:A:3500:MET:HE2	1.87	0.55
1:A:3770:LEU:O	1:A:3770:LEU:CG	2.53	0.55
1:A:2563:ALA:O	1:A:2804:ARG:NH1	2.40	0.55
1:A:4137:ASN:OD1	1:A:4138:LEU:N	2.40	0.55
1:A:1861:MET:HG2	1:A:1893:THR:HG21	1.88	0.54
2:C:362:LEU:HD23	2:C:376:LEU:HD12	1.89	0.54
1:A:1714:ALA:HB1	1:A:1853:VAL:HG22	1.90	0.54
1:A:1903:SER:OG	1:A:2018:MET:HE1	2.07	0.54
1:A:2107:ARG:NH2	1:A:2139:GLN:OE1	2.41	0.53
1:A:1897:GLU:O	1:A:1899:ARG:NH2	2.41	0.53
1:A:2210:LEU:HD11	1:A:2222:MET:HE2	1.90	0.53
1:A:2896:ARG:NH2	2:B:382:PHE:HE2	2.06	0.53
1:A:4300:ILE:N	1:A:4304:GLU:OE2	2.41	0.53
1:A:2979:VAL:HG21	1:A:2992:PHE:CZ	2.44	0.53
1:A:1842:MET:HE2	1:A:1861:MET:SD	2.49	0.53
1:A:2211:TYR:HB2	1:A:2237:LEU:HD11	1.91	0.53
1:A:4577:LEU:HD13	1:A:4635:PHE:CD1	2.44	0.53
1:A:3749:LEU:HD23	1:A:3770:LEU:HD12	1.89	0.53
1:A:1861:MET:HE2	1:A:1890:LEU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:THR:HG22	2:B:189:HIS:CD2	2.44	0.52
1:A:2896:ARG:HD2	2:B:340:TRP:CH2	2.45	0.52
1:A:2012:MET:SD	1:A:2013:ALA:N	2.82	0.52
1:A:2896:ARG:NH1	2:B:340:TRP:CZ3	2.77	0.52
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.42	0.52
1:A:2297:LYS:O	1:A:2338:ASN:ND2	2.44	0.51
1:A:2918:HIS:O	1:A:2922:ILE:HD12	2.10	0.51
1:A:2423:MET:HE1	1:A:2462:LEU:CD2	2.40	0.51
1:A:2517:TYR:CD2	1:A:2521:ILE:HD11	2.45	0.51
1:A:2066:ALA:HA	1:A:2069:ILE:HG22	1.92	0.51
2:B:293:ILE:HG21	2:B:310:PHE:CE2	2.45	0.51
1:A:4391:ILE:HD12	1:A:4479:VAL:HG11	1.93	0.51
1:A:2207:VAL:HG12	1:A:2237:LEU:HD12	1.93	0.50
1:A:2461:MET:HG2	1:A:2583:THR:HG21	1.93	0.50
1:A:2654:GLN:O	1:A:2705:ARG:NH2	2.45	0.50
1:A:2606:PHE:HE2	1:A:2617:VAL:HG11	1.76	0.50
1:A:3758:GLY:O	1:A:3759:ARG:C	2.54	0.50
1:A:2943:LYS:NZ	3:A:4704:ADP:O1B	2.43	0.50
2:B:313:SER:OG	2:B:323:TRP:NE1	2.45	0.50
2:B:366:ASP:CB	2:B:373:MET:HE3	2.42	0.49
1:A:1873:LEU:O	1:A:1876:GLN:NE2	2.37	0.49
2:B:171:ASP:O	2:B:173:THR:HG23	2.12	0.49
1:A:3821:ILE:HD11	1:A:4345:LYS:HB2	1.94	0.49
2:C:379:HIS:CG	2:C:399:SER:OG	2.65	0.49
1:A:4042:LEU:N	1:A:4143:ARG:O	2.45	0.49
1:A:2581:LEU:HD22	1:A:2591:LEU:HD21	1.93	0.49
1:A:4050:ASP:OD2	1:A:4050:ASP:N	2.46	0.49
1:A:2573:ASP:O	1:A:2577:HIS:ND1	2.46	0.48
1:A:4388:LEU:CD2	1:A:4431:LEU:HD22	2.43	0.48
1:A:4388:LEU:HD22	1:A:4431:LEU:HD22	1.95	0.48
1:A:2892:TYR:CE1	2:B:339:ASN:ND2	2.77	0.48
1:A:3154:LEU:HD23	1:A:3171:ILE:HG23	1.95	0.48
1:A:3872:ALA:O	1:A:3880:HIS:NE2	2.45	0.48
1:A:3096:ASP:OD1	1:A:3097:TRP:N	2.46	0.48
1:A:2975:ASP:O	1:A:2979:VAL:HG12	2.13	0.48
1:A:1805:ARG:NH1	1:A:1809:GLU:OE2	2.46	0.48
2:B:318:LYS:HB3	2:B:337:HIS:O	2.14	0.48
1:A:4293:ASP:N	1:A:4293:ASP:OD1	2.46	0.47
1:A:4323:LEU:HD12	1:A:4324:PRO:HD2	1.95	0.47
1:A:4481:ASP:OD2	1:A:4485:ARG:NH1	2.45	0.47
1:A:2047:GLN:NE2	1:A:2067:ASN:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:LEU:CD1	1:A:1749:LEU:HD21	2.44	0.47
1:A:4041:VAL:HG11	1:A:4125:PHE:CE2	2.50	0.47
2:B:316:ARG:HD3	2:B:340:TRP:CE2	2.49	0.47
1:A:2697:ASP:OD1	1:A:2699:THR:HG22	2.15	0.47
1:A:3478:LEU:CD2	1:A:3767:ILE:HG12	2.45	0.46
1:A:3824:LEU:O	1:A:4139:LEU:HD23	2.15	0.46
2:B:293:ILE:HD13	2:B:310:PHE:CD2	2.50	0.46
1:A:1861:MET:HG3	1:A:1862:ALA:N	2.30	0.46
2:C:169:SER:OG	2:C:171:ASP:OD1	2.33	0.46
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	1.97	0.46
2:C:217:LYS:HG3	2:C:229:THR:HG23	1.96	0.46
1:A:2614:ASP:OD1	1:A:2614:ASP:N	2.49	0.46
1:A:2075:LEU:HD23	1:A:2078:GLU:OE2	2.15	0.46
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.33	0.46
1:A:3817:SER:HB2	1:A:4346:MET:HE1	1.98	0.46
1:A:1831:ASP:OD1	1:A:1832:ASN:N	2.48	0.46
1:A:2237:LEU:HD22	1:A:2300:TRP:HH2	1.82	0.45
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.47	0.45
1:A:2813:LEU:HD22	1:A:2816:LEU:HD11	1.98	0.45
1:A:2919:VAL:HG13	1:A:2950:VAL:HG22	1.98	0.45
2:B:136:ASP:O	2:B:140:GLY:N	2.49	0.45
2:C:108:ARG:O	2:C:109:SER:OG	2.33	0.45
1:A:3110:THR:O	1:A:3140:ARG:NH1	2.50	0.45
2:C:96:PRO:HB2	2:C:376:LEU:HD11	2.00	0.44
1:A:1972:SER:HA	1:A:1975:VAL:HG12	1.98	0.44
1:A:2432:LEU:HD13	1:A:2522:THR:HB	1.98	0.44
1:A:4577:LEU:HD11	1:A:4638:ARG:HD3	1.98	0.44
1:A:2912:PHE:O	1:A:2915:VAL:HG12	2.18	0.44
2:C:399:SER:C	2:C:401:ASP:N	2.73	0.44
2:C:93:GLU:N	2:C:93:GLU:OE2	2.51	0.44
1:A:2444:GLU:OE1	1:A:2444:GLU:N	2.45	0.44
2:B:366:ASP:OD2	2:B:369:ASN:ND2	2.51	0.44
2:C:243:ASN:OD1	2:C:246:GLY:N	2.51	0.44
1:A:2499:LEU:HD23	1:A:2514:LEU:HD22	1.99	0.44
2:C:117:HIS:NE2	2:C:162:GLY:O	2.49	0.44
1:A:2668:LEU:HD21	1:A:2720:ARG:HA	2.00	0.43
2:B:316:ARG:HD3	2:B:340:TRP:CD2	2.52	0.43
1:A:2221:MET:CE	1:A:2348:LEU:HD21	2.48	0.43
1:A:3824:LEU:HD13	1:A:4130:ILE:HG23	1.99	0.43
1:A:1751:VAL:HG13	1:A:1814:GLU:OE1	2.19	0.43
1:A:2090:LEU:HD23	3:A:4701:ADP:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2581:LEU:CD2	1:A:2591:LEU:HD21	2.47	0.43
1:A:1713:LEU:HD11	1:A:1749:LEU:HD21	2.01	0.43
1:A:2785:THR:OG1	1:A:2786:GLN:N	2.51	0.43
1:A:3691:ASP:OD1	1:A:3692:LEU:N	2.50	0.43
1:A:2964:HIS:ND1	1:A:2965:ARG:O	2.51	0.43
1:A:2203:TRP:O	1:A:2207:VAL:HG23	2.18	0.43
2:C:366:ASP:OD2	2:C:369:ASN:ND2	2.49	0.43
1:A:3931:GLN:NE2	1:A:3996:PHE:O	2.46	0.43
1:A:4105:TRP:CH2	1:A:4109:LEU:HD21	2.54	0.43
1:A:2694:ARG:NH2	1:A:2697:ASP:OD2	2.52	0.42
1:A:3114:ASP:HB3	2:C:185:ILE:O	2.19	0.42
2:B:172:MET:HE1	2:B:194:ASN:N	2.33	0.42
2:C:124:VAL:HG12	2:C:134:VAL:HG22	2.01	0.42
1:A:3586:TYR:O	1:A:3696:VAL:HG13	2.19	0.42
2:B:210:ALA:HB1	2:B:237:VAL:HB	2.01	0.42
2:C:216:ILE:O	2:C:230:PHE:N	2.49	0.42
1:A:2996:GLU:HB3	1:A:3068:MET:HE1	2.01	0.42
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.47	0.42
1:A:3478:LEU:HD12	1:A:3478:LEU:O	2.19	0.42
2:C:231:THR:OG1	2:C:232:GLY:N	2.52	0.42
1:A:4042:LEU:HD22	1:A:4128:MET:HE3	2.02	0.42
1:A:2458:LEU:HD12	1:A:2497:ALA:HB1	2.02	0.42
2:B:159:ASP:OD1	2:B:160:HIS:N	2.51	0.42
2:B:257:THR:OG1	2:B:273:ARG:HG2	2.20	0.42
1:A:2453:ARG:NH2	1:A:2505:ASP:OD2	2.53	0.41
1:A:3696:VAL:HG12	1:A:3697:THR:O	2.19	0.41
1:A:4474:THR:OG1	1:A:4475:VAL:N	2.53	0.41
2:C:92:LYS:N	2:C:93:GLU:OE2	2.53	0.41
2:B:176:LEU:O	2:B:185:ILE:N	2.53	0.41
1:A:2576:ARG:O	1:A:2580:LEU:HD23	2.20	0.41
1:A:1860:GLN:O	1:A:1861:MET:HB2	2.20	0.41
2:B:157:SER:O	2:B:165:LEU:HD12	2.20	0.41
1:A:1959:GLU:OE1	1:A:2025:ARG:NH1	2.49	0.41
2:B:183:GLU:OE1	2:B:184:CYS:N	2.50	0.41
2:C:384:THR:HB	2:C:398:GLY:O	2.20	0.41
2:C:124:VAL:HG23	2:C:156:ILE:HD12	2.03	0.41
2:C:271:GLU:N	2:C:271:GLU:OE1	2.53	0.41
1:A:2037:ARG:NH2	1:A:4214:SER:OG	2.53	0.41
2:B:319:THR:HG22	2:B:335:VAL:HG22	2.01	0.41
1:A:2934:LEU:HD11	1:A:3068:MET:HG2	2.02	0.41
1:A:2979:VAL:HG21	1:A:2992:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3620:ARG:NH2	1:A:3644:VAL:HG11	2.36	0.41
1:A:1930:PHE:HD1	1:A:2326:THR:HG21	1.86	0.41
1:A:1713:LEU:HD21	1:A:1748:GLN:HE21	1.86	0.40
1:A:4055:VAL:HG11	1:A:4095:MET:SD	2.61	0.40
2:C:171:ASP:O	2:C:173:THR:HG23	2.21	0.40
2:C:254:ASN:HA	2:C:278:VAL:HG13	2.03	0.40
1:A:3478:LEU:HD22	1:A:3767:ILE:HG12	2.04	0.40
2:C:150:THR:OG1	2:C:171:ASP:OD2	2.34	0.40
1:A:2896:ARG:NH2	2:B:382:PHE:CE2	2.88	0.40
2:C:172:MET:HE1	2:C:193:HIS:C	2.46	0.40
1:A:2195:ASP:OD1	1:A:2198:GLU:N	2.53	0.40
1:A:2202:MET:SD	1:A:2202:MET:N	2.91	0.40
1:A:2871:ILE:HD12	1:A:2871:ILE:H	1.86	0.40
2:C:139:THR:O	2:C:139:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2522/3328 (76%)	2457 (97%)	65 (3%)	0	100	100
2	B	300/411 (73%)	278 (93%)	22 (7%)	0	100	100
2	C	300/411 (73%)	288 (96%)	11 (4%)	1 (0%)	36	70
All	All	3122/4150 (75%)	3023 (97%)	98 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	400	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2034/2953 (69%)	2031 (100%)	3 (0%)	88	89
2	B	267/364 (73%)	265 (99%)	2 (1%)	76	79
2	C	257/364 (71%)	256 (100%)	1 (0%)	84	84
All	All	2558/3681 (70%)	2552 (100%)	6 (0%)	85	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2087	ASP
1	A	3207	LYS
1	A	3766	ILE
2	B	149	HIS
2	B	318	LYS
2	C	107	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2346	GLN
1	A	2439	HIS
1	A	2698	GLN
1	A	2827	HIS
1	A	3014	ASN
1	A	3152	GLN
1	A	3185	ASN
1	A	3523	GLN
1	A	3526	GLN
1	A	3527	ASN
1	A	4100	HIS
2	B	206	HIS
2	B	277	HIS
2	C	275	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	4701	-	28,29,29	1.36	4 (14%)	43,45,45	1.89	9 (20%)
4	ATP	A	4702	-	32,33,33	0.31	0	48,52,52	0.67	0
3	ADP	A	4704	-	28,29,29	1.34	4 (14%)	43,45,45	1.86	11 (25%)
3	ADP	A	4703	-	28,29,29	0.46	0	43,45,45	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4701	-	-	0/16/32/32	0/3/3/3
4	ATP	A	4702	-	-	3/22/38/38	0/3/3/3
3	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
3	ADP	A	4703	-	-	4/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4704	ADP	C5-C4	4.39	1.46	1.39
3	A	4701	ADP	C5-C4	4.35	1.46	1.39
3	A	4704	ADP	C5-C6	2.55	1.48	1.41
3	A	4701	ADP	C5-N7	-2.46	1.34	1.39
3	A	4704	ADP	C5-N7	-2.44	1.34	1.39
3	A	4701	ADP	C5-C6	2.44	1.47	1.41
3	A	4704	ADP	C8-N7	2.32	1.36	1.31
3	A	4701	ADP	C8-N7	2.19	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4701	ADP	C5-C4-N3	-5.91	118.57	126.72
3	A	4704	ADP	C5-C4-N3	-5.54	119.09	126.72
3	A	4701	ADP	N3-C4-N9	4.92	135.53	127.17
3	A	4704	ADP	N3-C4-N9	4.36	134.58	127.17
3	A	4701	ADP	C2-N3-C4	3.85	121.22	111.83
3	A	4704	ADP	N3-C2-N1	-3.81	122.81	128.58
3	A	4704	ADP	C2-N3-C4	3.77	121.04	111.83
3	A	4701	ADP	N3-C2-N1	-3.63	123.09	128.58
3	A	4704	ADP	C4-C5-N7	-3.39	106.70	110.58
3	A	4701	ADP	C4-C5-N7	-3.17	106.96	110.58
3	A	4701	ADP	C4-N9-C8	3.10	108.99	105.74
3	A	4704	ADP	C4-N9-C8	2.81	108.69	105.74
3	A	4704	ADP	C5-N7-C8	2.67	107.64	103.45
3	A	4704	ADP	C3'-C2'-C1'	2.65	106.48	101.46
3	A	4701	ADP	C5-N7-C8	2.62	107.57	103.45
3	A	4701	ADP	N9-C8-N7	-2.36	110.58	113.94
3	A	4704	ADP	N9-C8-N7	-2.32	110.64	113.94
3	A	4704	ADP	C2-N1-C6	2.24	122.40	118.73
3	A	4704	ADP	C6-C5-N7	2.15	136.23	132.09
3	A	4701	ADP	C3'-C2'-C1'	2.08	105.39	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4703	ADP	PA-O3A-PB-O2B
3	A	4704	ADP	O4'-C4'-C5'-O5'
3	A	4704	ADP	C3'-C4'-C5'-O5'
4	A	4702	ATP	O4'-C4'-C5'-O5'

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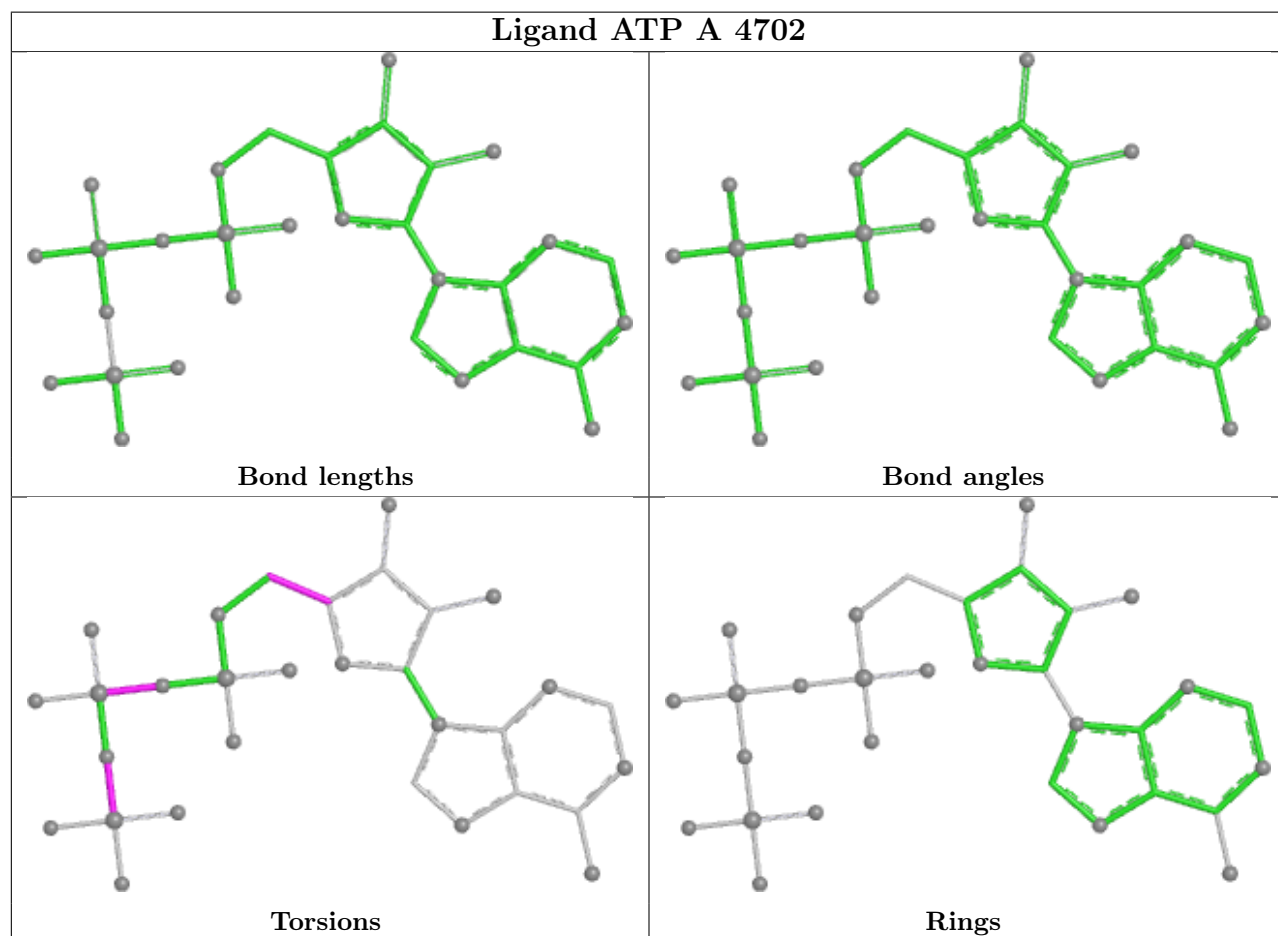
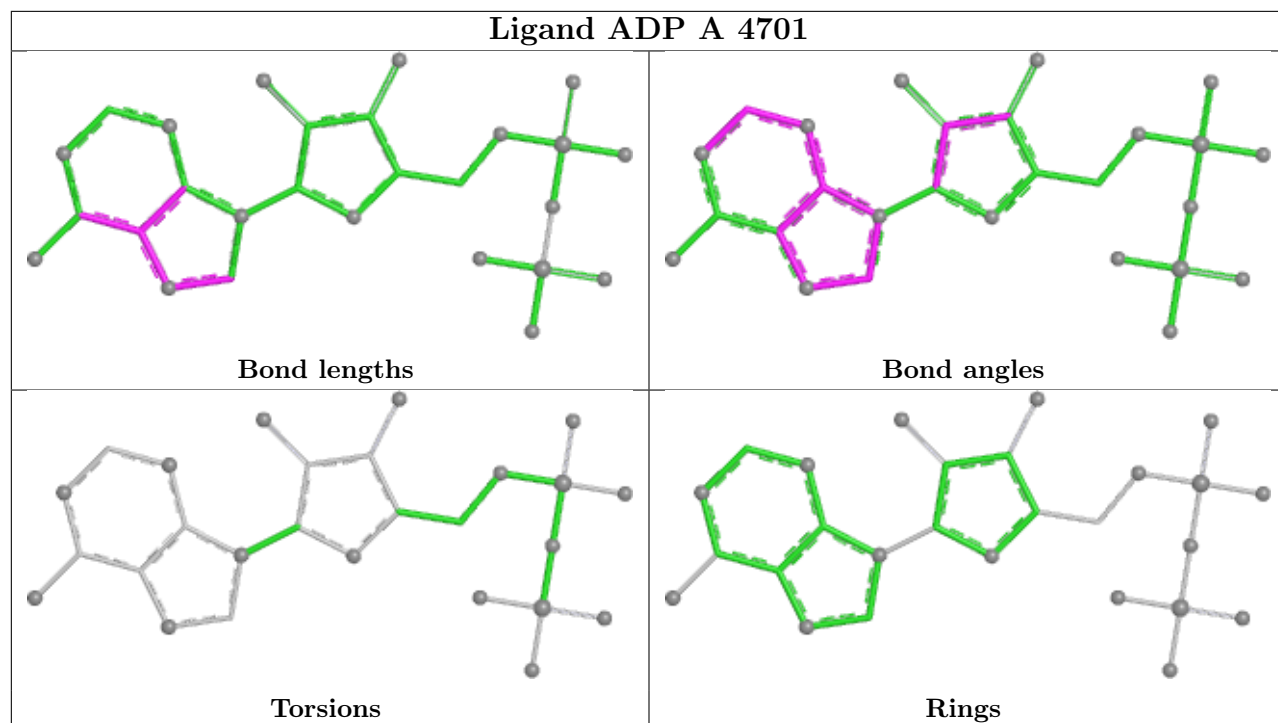
Mol	Chain	Res	Type	Atoms
3	A	4703	ADP	C4'-C5'-O5'-PA
4	A	4702	ATP	PA-O3A-PB-O2B
3	A	4703	ADP	O4'-C4'-C5'-O5'
4	A	4702	ATP	PB-O3B-PG-O2G
3	A	4703	ADP	C3'-C4'-C5'-O5'
3	A	4704	ADP	PB-O3A-PA-O2A

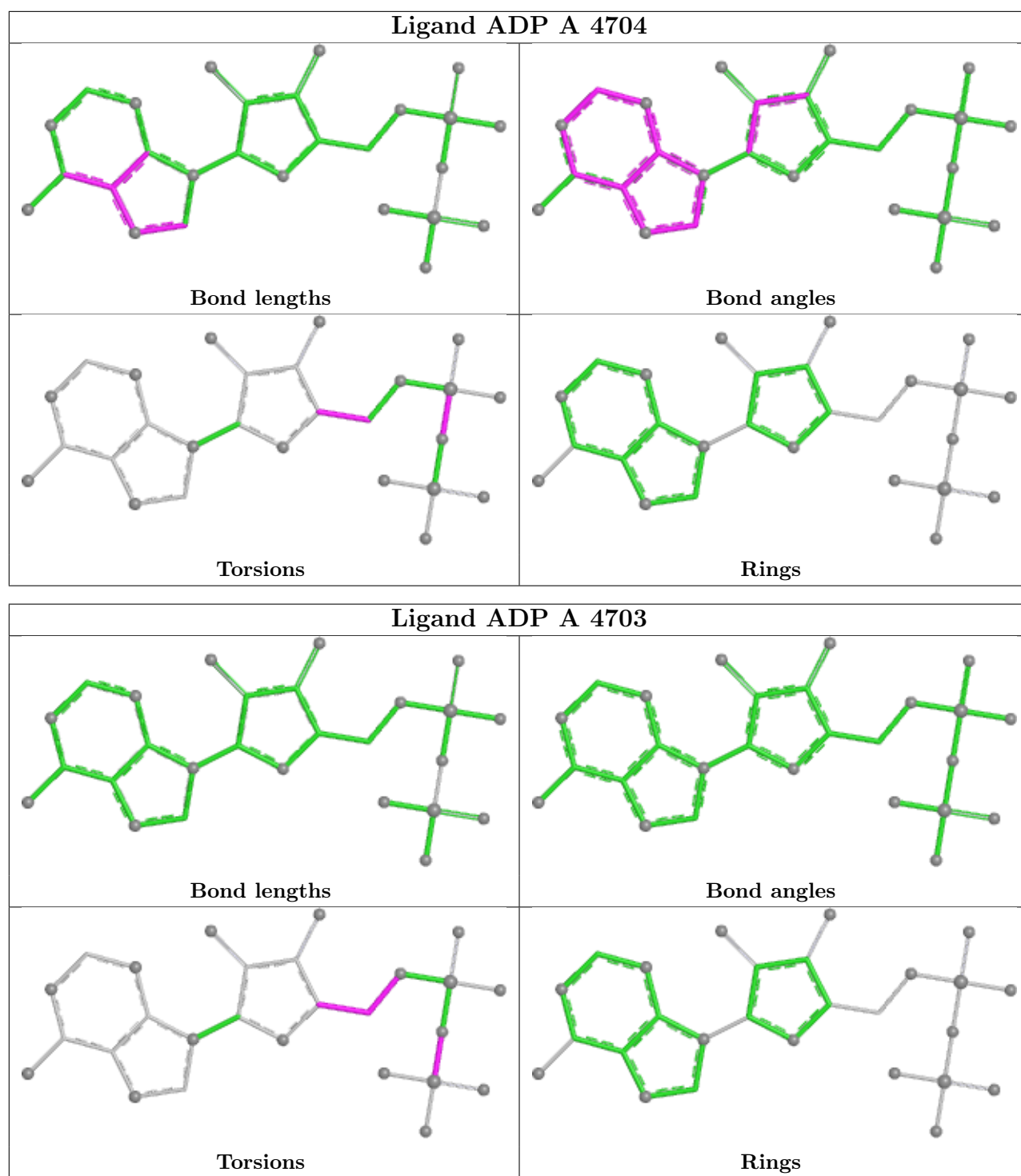
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4701	ADP	1	0
3	A	4704	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

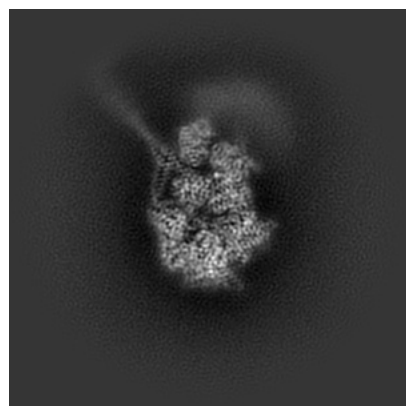
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27782. These allow visual inspection of the internal detail of the map and identification of artifacts.

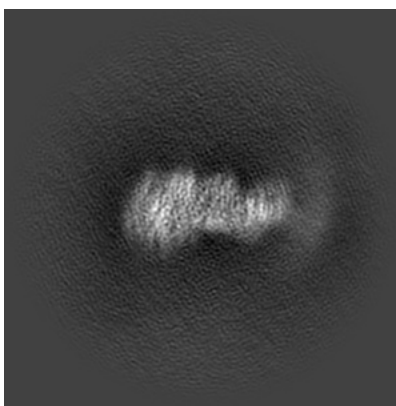
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

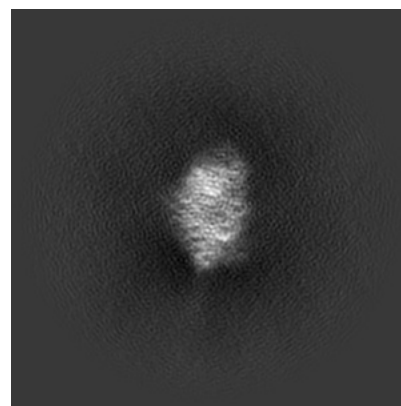
6.1.1 Primary map



X

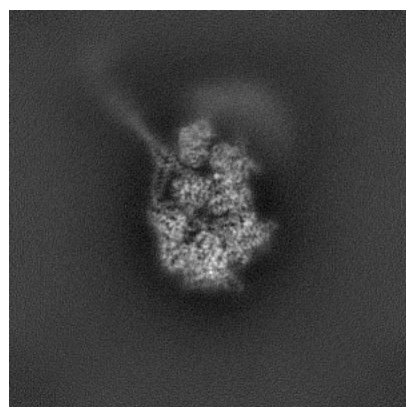


Y

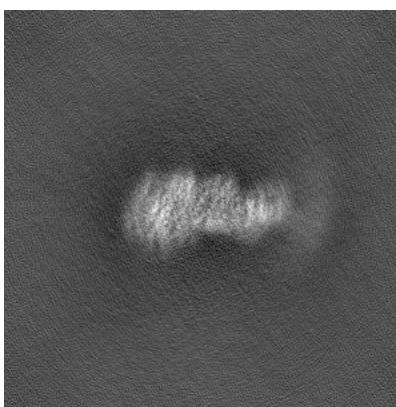


Z

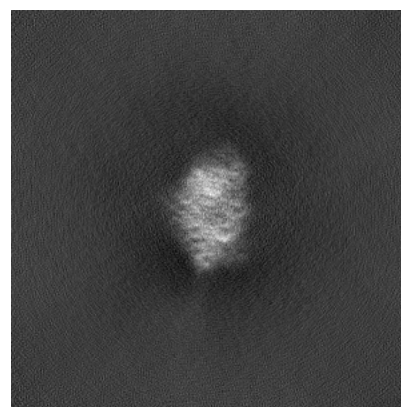
6.1.2 Raw map



X



Y

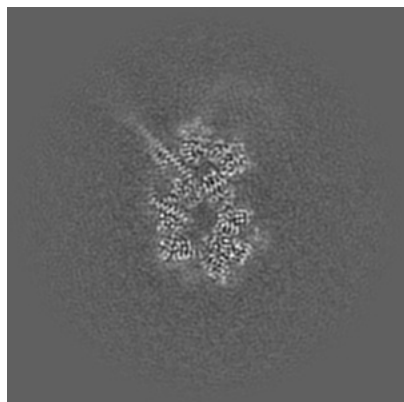


Z

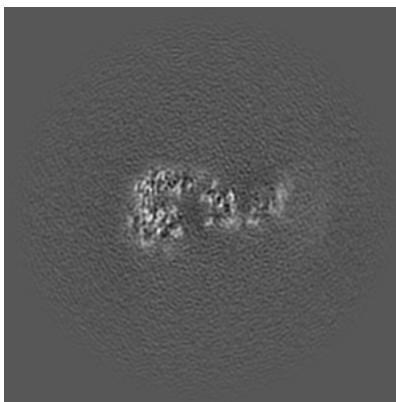
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

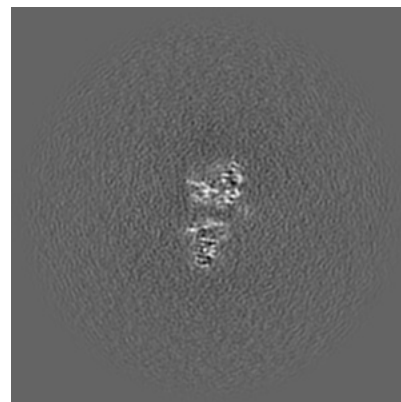
6.2.1 Primary map



X Index: 176

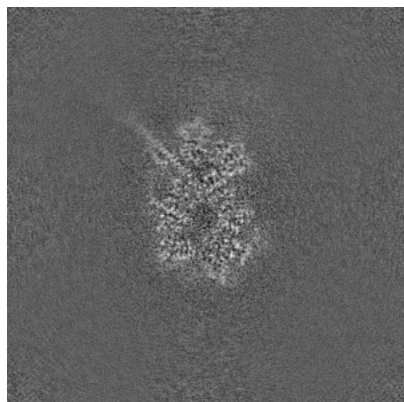


Y Index: 176

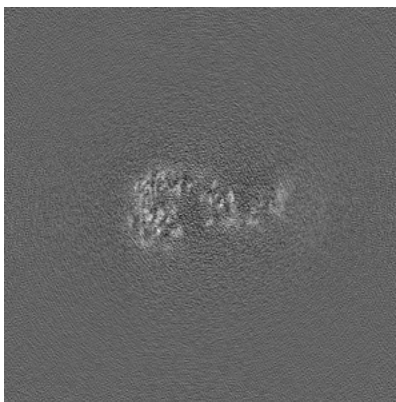


Z Index: 176

6.2.2 Raw map



X Index: 176



Y Index: 176

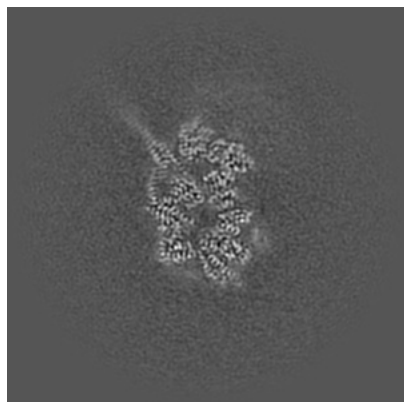


Z Index: 176

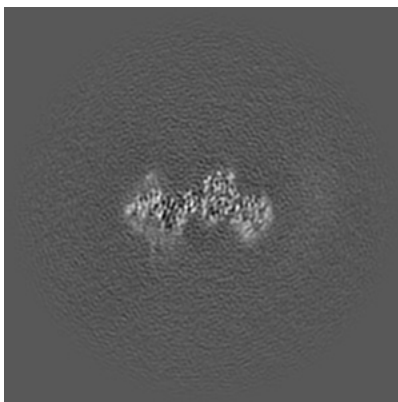
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

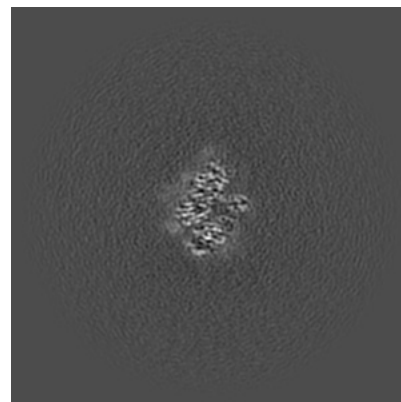
6.3.1 Primary map



X Index: 174

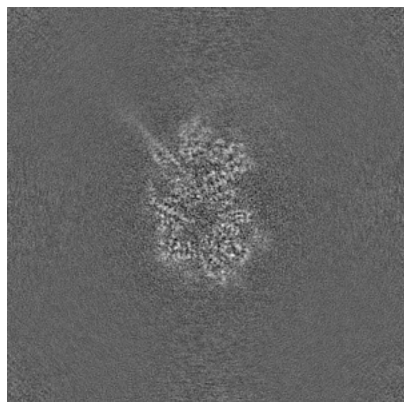


Y Index: 190

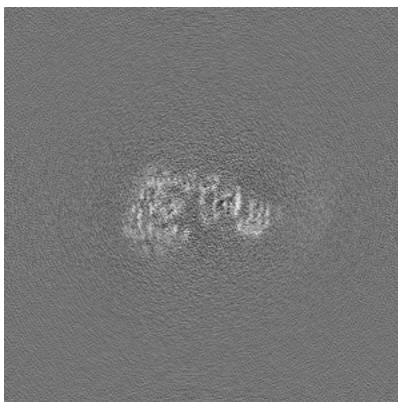


Z Index: 140

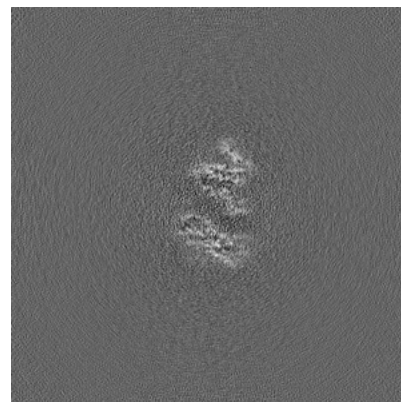
6.3.2 Raw map



X Index: 175



Y Index: 182

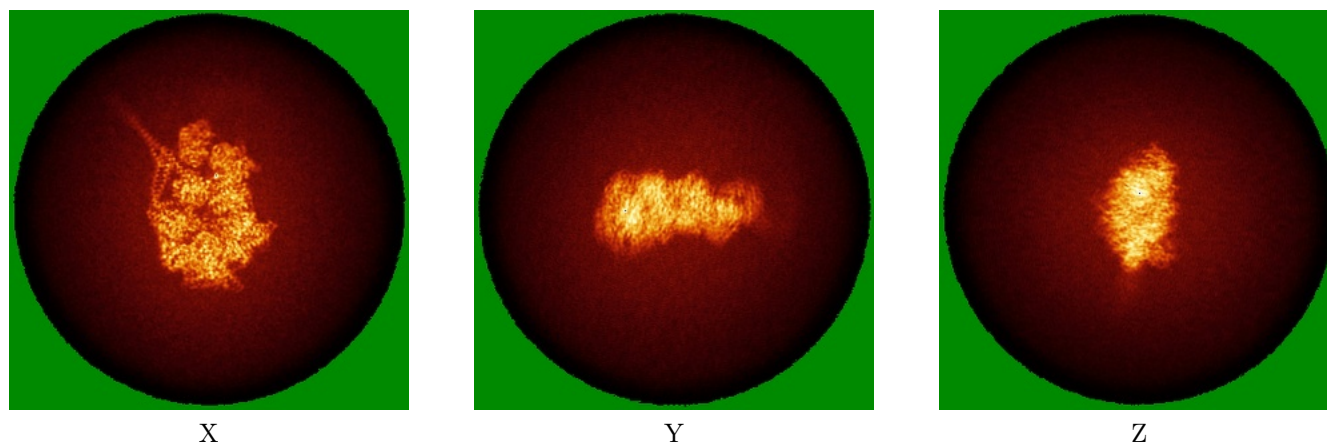


Z Index: 163

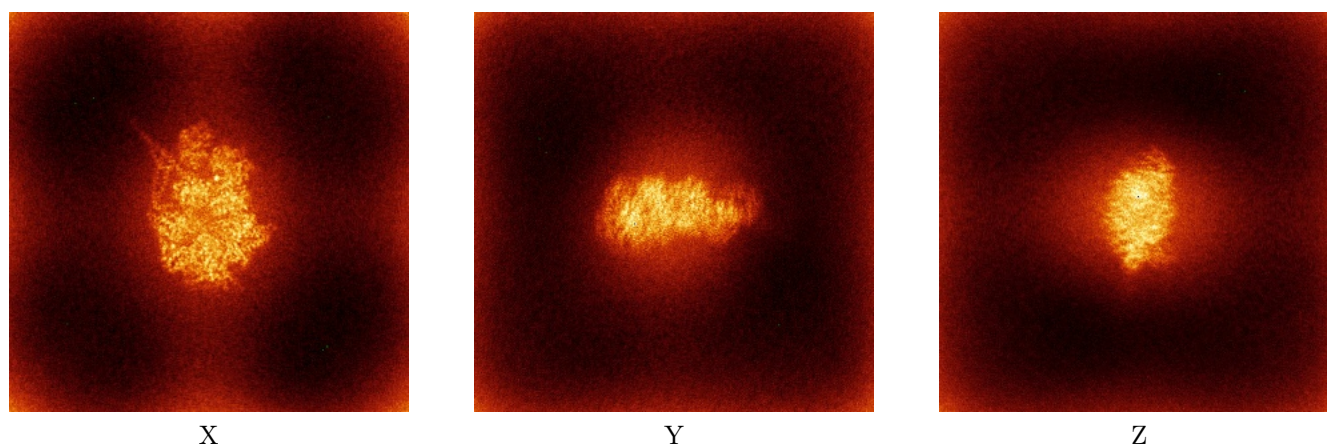
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

This section was not generated.

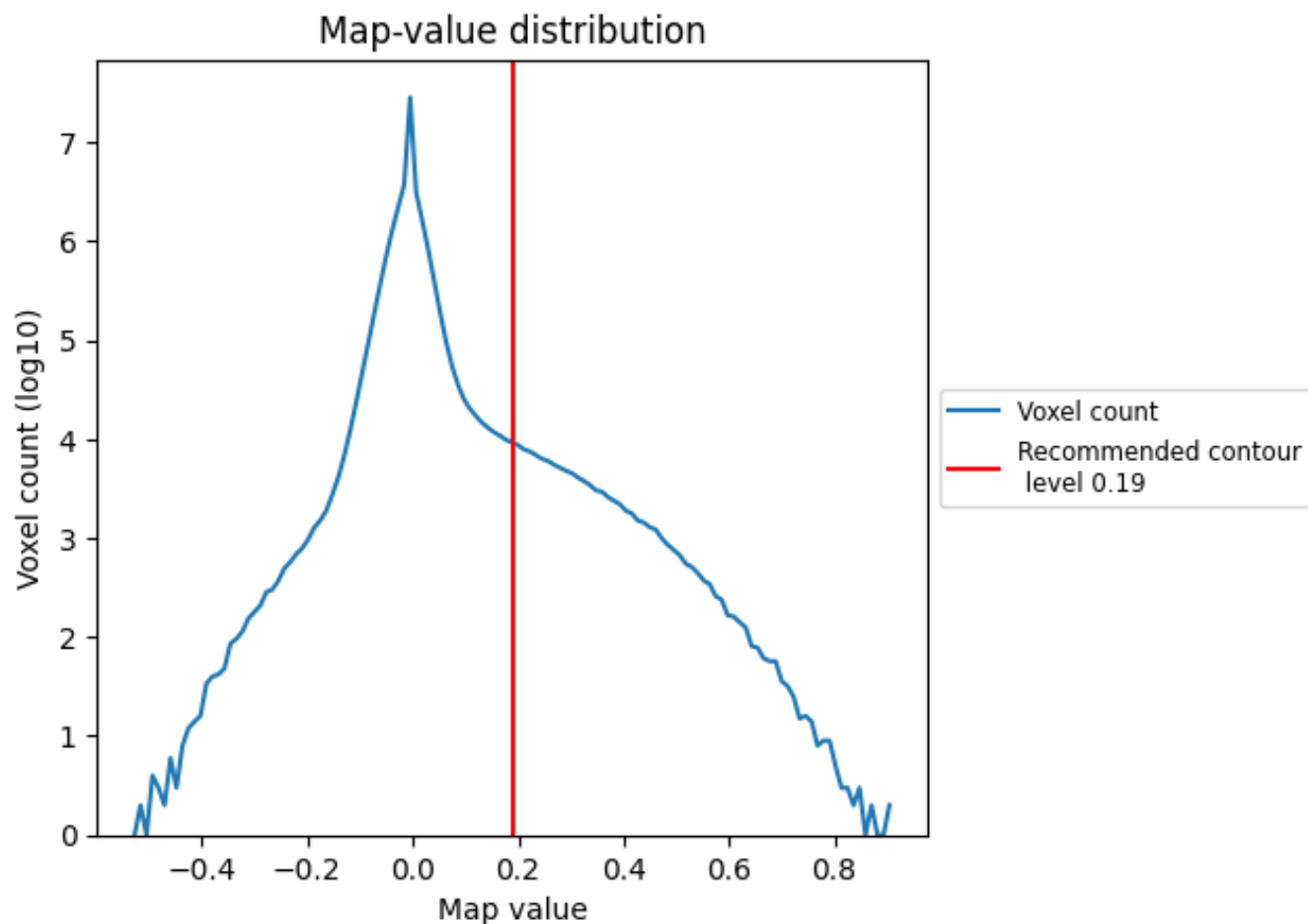
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

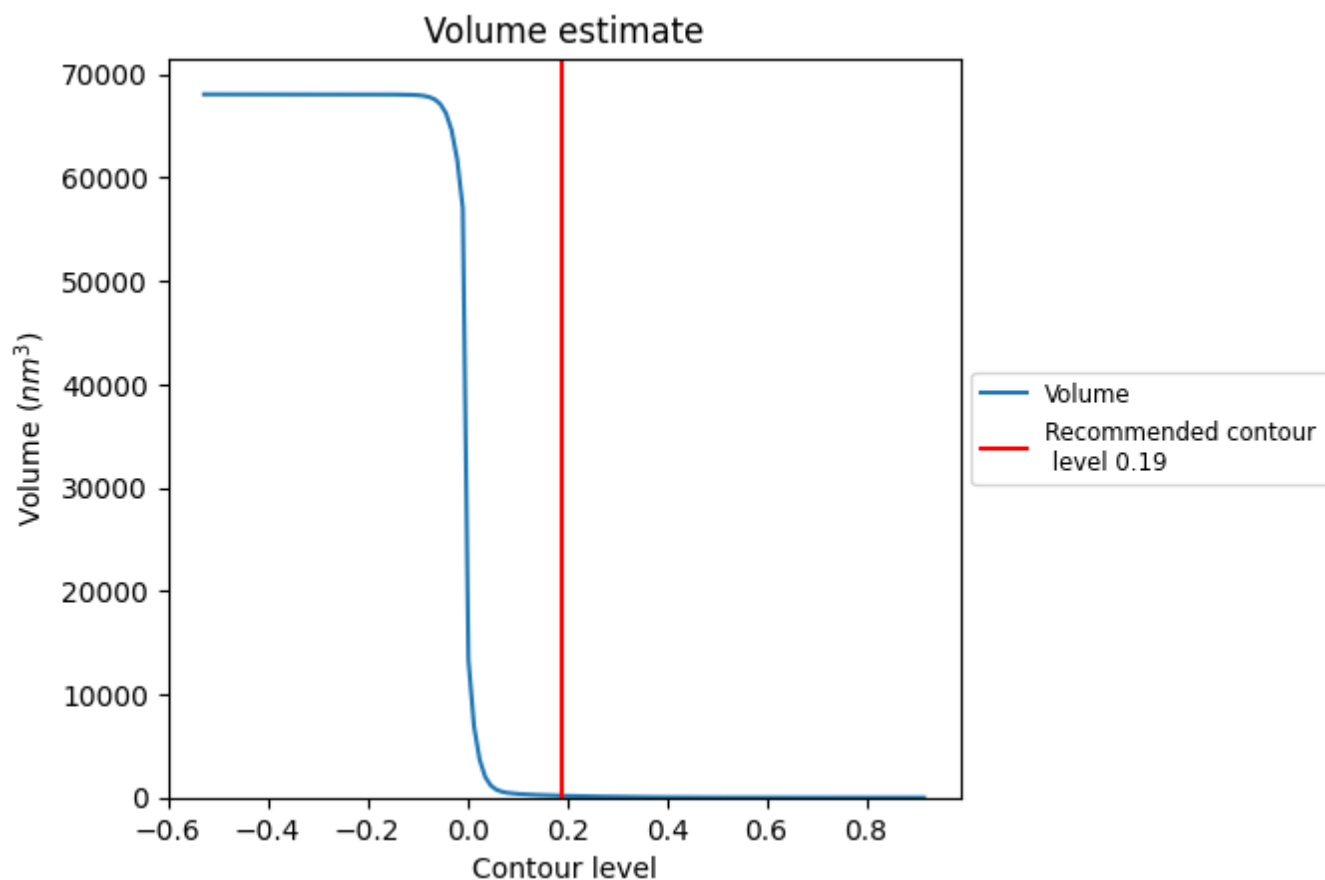
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

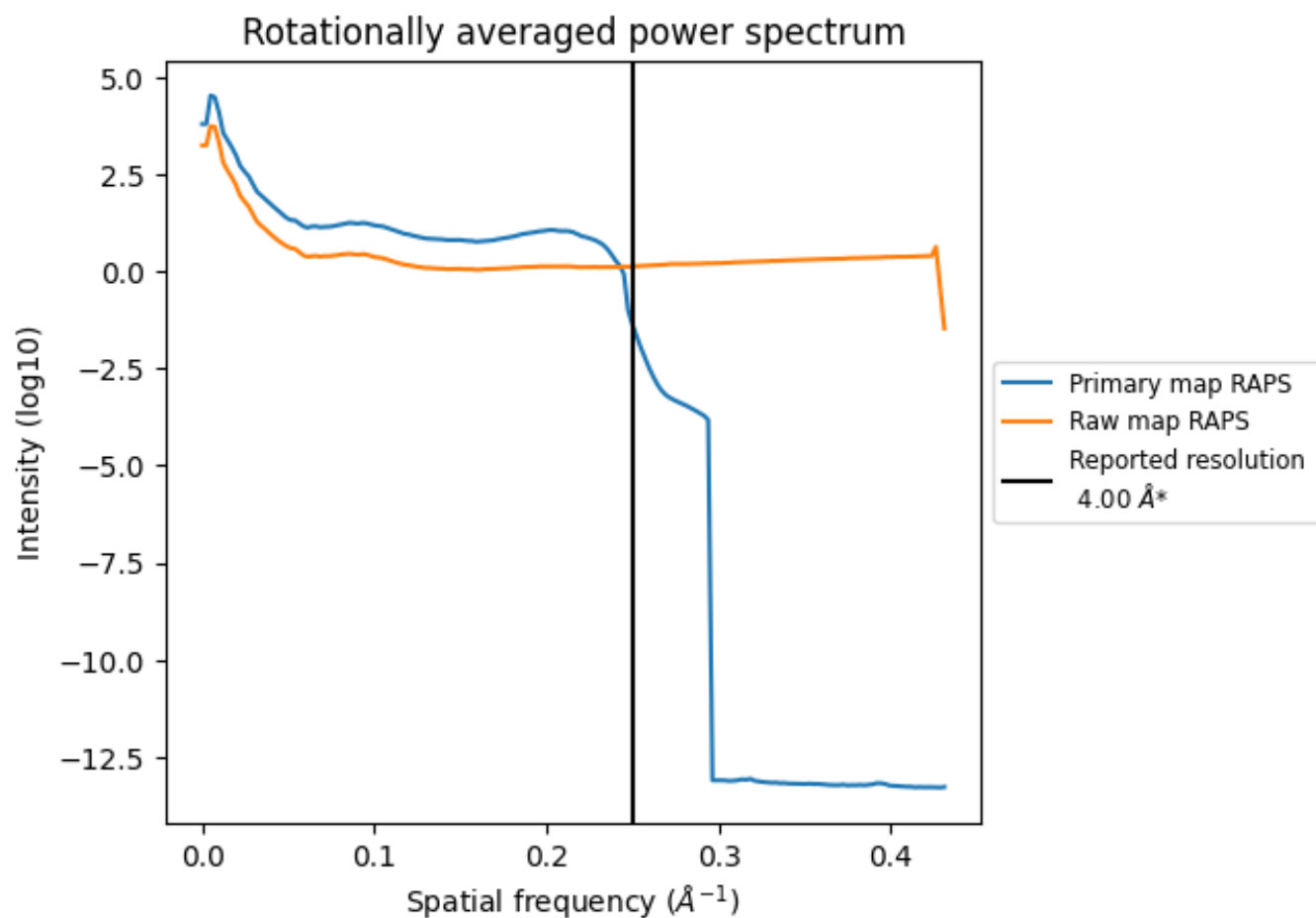
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; this corresponds to an approximate mass of 157 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

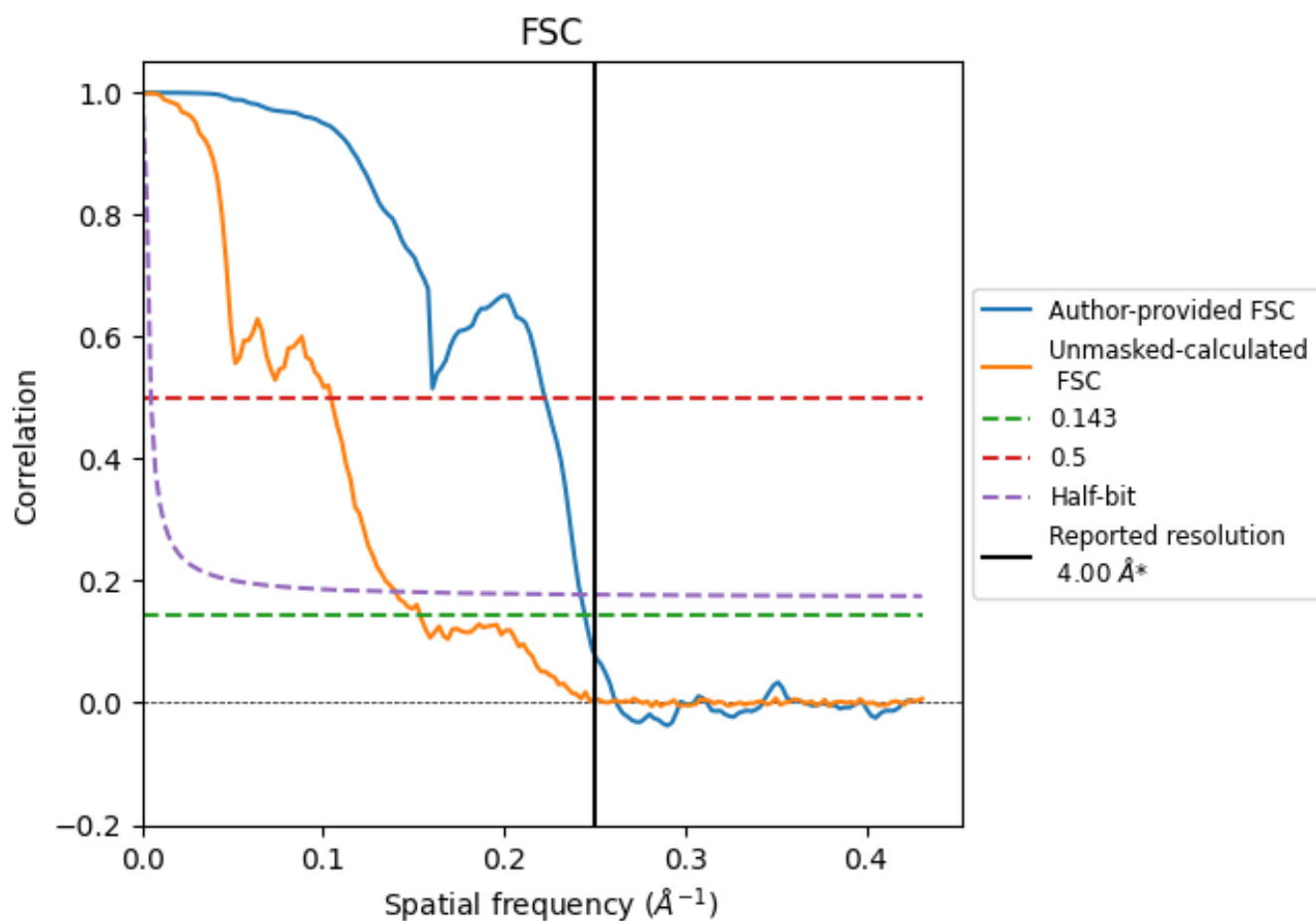


*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.09	4.49	4.13
Unmasked-calculated*	6.51	9.59	7.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.51 differs from the reported value 4.0 by more than 10 %

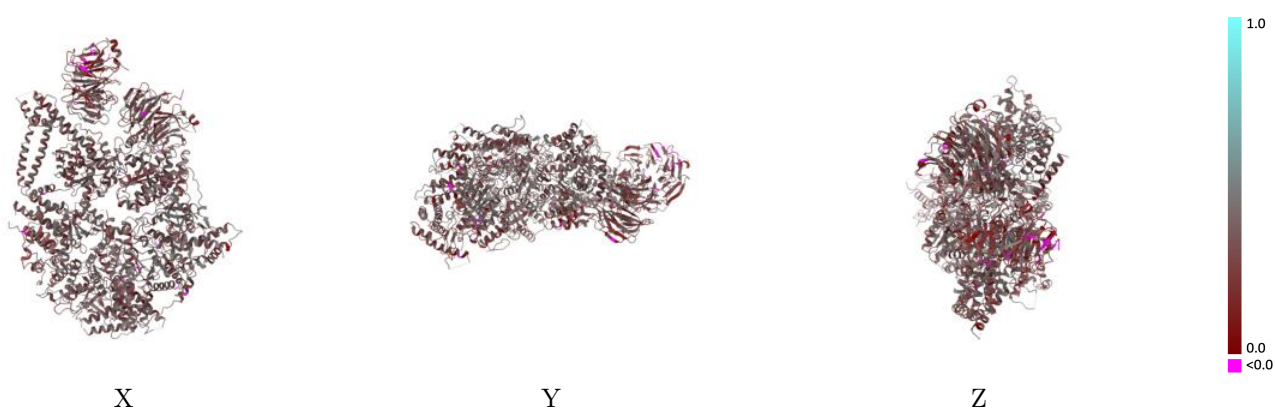
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27782 and PDB model 8DYU. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

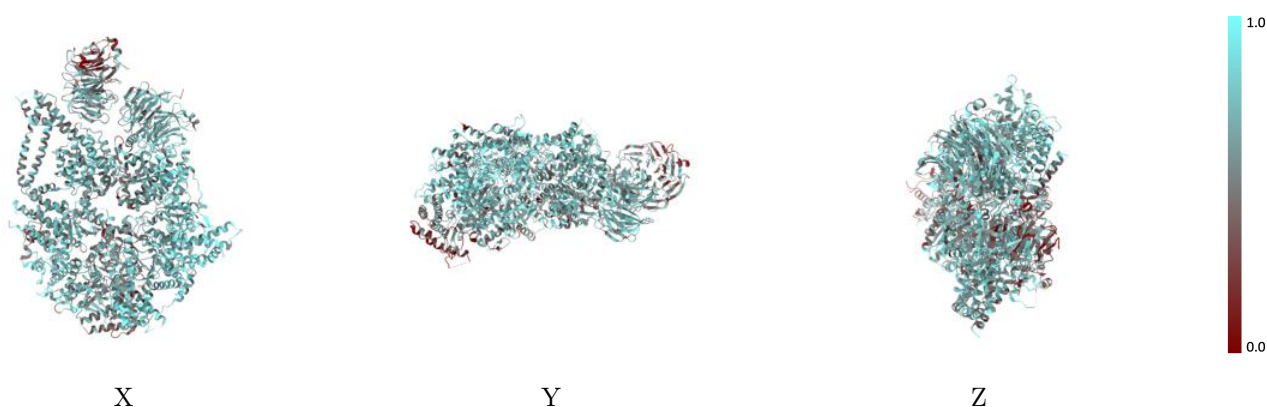
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



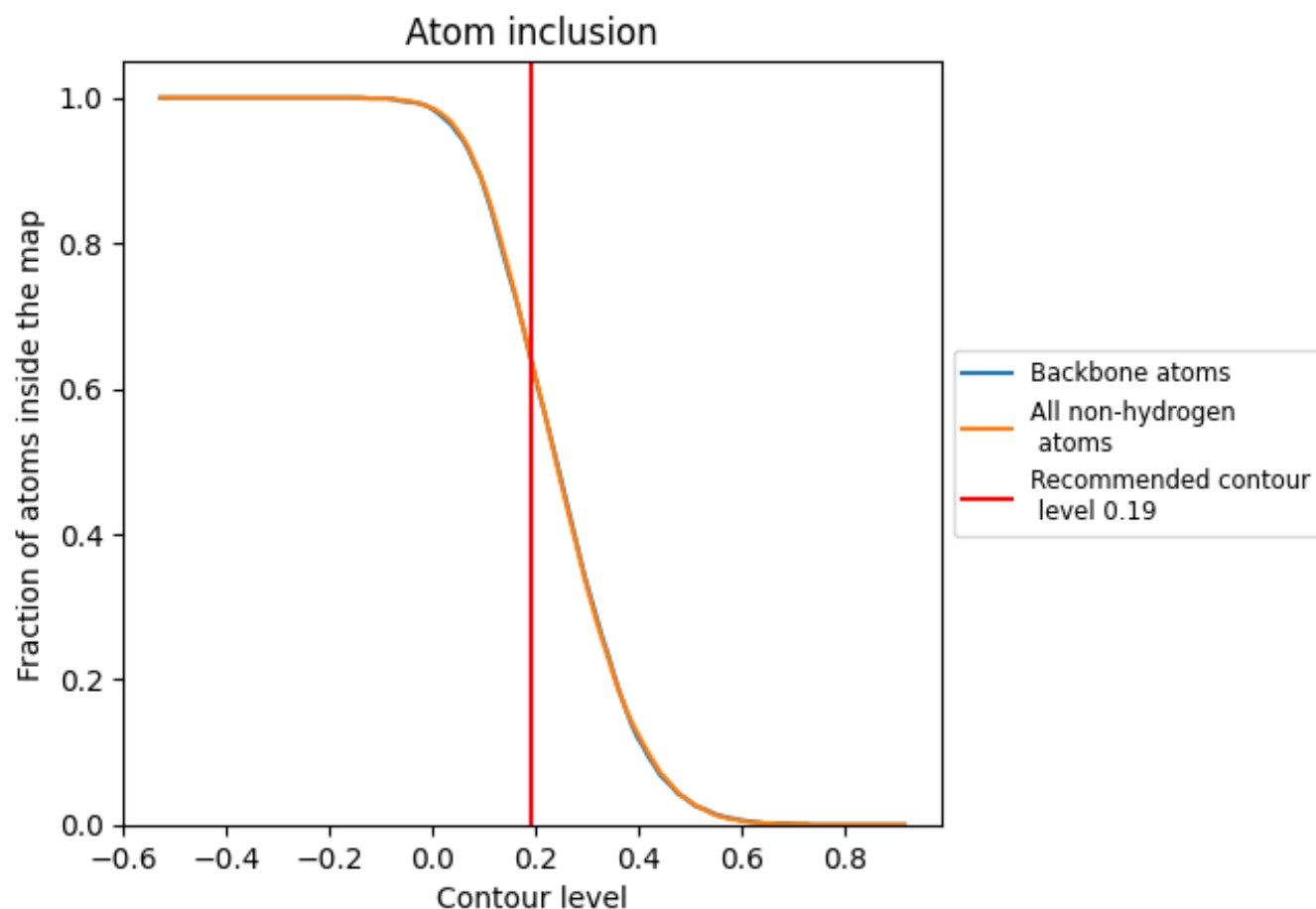
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.3390
A	0.6720	0.3510
B	0.6730	0.3140
C	0.5200	0.2670

